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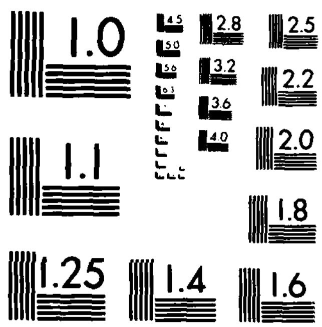

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A TWO-DIMENSIONAL SMOOTHING SPLINE AND A REGRESSION PROBLEM

M. ROSENBLATT

INTRODUCTION

Splines have been proposed in a variety of approximation problems in recent years (see SCHOENBERG [4]). Smoothing splines as a particular subclass of these have drawn particular attention (see WAHBA [5]) in the context of a set of regression problems. It had also been noted that boundary effects like Gibbs effects can arise in the case of natural splines (see ROSENBLATT [3]). A few remarks will be made about a simple one-dimensional regression problem. Suppose that observations

$$x_j = f(t_j) + \varepsilon_j \ , \ t_j = j/n \ , \ j = 0, 1, \ldots, n-1 \ ,$$

are made and that f is an unknown smooth function with

the ϵ_i random errors

$$E\epsilon_i \equiv 0$$

$$E\epsilon_j\epsilon_k = \delta_{jk}\sigma^2 .$$

A cubic smoothing spline estimate $g(t;\lambda)$ of $f(t)$ is a function that minimizes

$$(1) \qquad \frac{1}{n}\sum_{i=1}^{n} [x_i - g(t_i)]^2 + \lambda \int (g''(t))^2 dt .$$

The asymptotic behavior of such an estimate g of f in terms of the mean square error

$$(2) \qquad E|g(t;\lambda) - f(t)|^2$$

has been examined as $n \to \infty$. One determines the rate at which the parameter $\lambda = \lambda(n) \downarrow 0$ as $n \to \infty$ so as to make (2) go to zero as fast as possible under the smoothness assumptions made on f. The case of a periodic function f and a periodic smoothing spline has been discussed in WAHBA [5] and RICE and ROSENBLATT [1]. In the latter paper it has been shown that boundary effects can even arise in the case of periodic smoothing splines. The non-periodic case of a smoothing spline is treated in RICE and ROSENBLATT [2]. The boundary effects of a nonperiodic

cubic spline are examined in some detail in this last paper.

There are many measures analogous to (1) that one could consider in the two dimensional case. We shall not consider one that leads to a doubly cubic spline but rather a simpler one. Let us consider observations

$$x_{j,k} = f(t_j, s_k) + \epsilon_{j,k}$$

$$t_j = j/n, s_k = k/n ,$$

$$j,k = 0,1,\dots,n-1$$

with f an unknown smooth function and the $\epsilon_{j,k}$ random errors with

$$E\epsilon_{j,k} \equiv 0$$

$$E\epsilon_{j,k}\epsilon_{j',k'} = \delta_{j,j'}\,\delta_{k,k'}\,\sigma^2 .$$

The measure that will be minimized to obtain the smoothing spline approximation $g(t,s;\lambda)$ to f is

$$(3) \qquad \frac{1}{n^2}\sum_{j,k=0}^{n-1}[g(t_j,s_k)-x_{j,k}]^2 + {}$$

$$+ \frac{\lambda}{(2\pi)^2}\int_0^1\int_0^1 ((D_t g)^2 + (D_s f)^2)\,dt\,ds$$

with D_t and D_s the partial derivatives with respect to t and s respectively.

THE SMOOTHING SPLINE. For the sake of simplicity we shall basically consider the periodic situation. Let us first note that if f is continuously differentiable up to second order $(f \in C^2)$ for $k \neq 0$

$$f_{j,k} = \int_0^1 \int_0^1 \exp\{-2\pi i j t - 2\pi i k \tau\} f(t,\tau)\, dt\, d\tau =$$

$$= \frac{1}{-2\pi i k} \int_0^1 e^{-2\pi i j t} \{f(t,1) - f(t,0)\}\, dt -$$

$$- \frac{1}{(2\pi i k)^2} \int_0^1 e^{-2\pi i j t} \{D_\tau f(t,1) - D_\tau f(t,0)\}\, dt +$$

$$+ \frac{1}{(2\pi i k)^2} \int_0^1 \int_0^1 e^{-2\pi i j t - 2\pi i k \tau} D_\tau^2 f(t,\tau)\, dt\, d\tau .$$

The corresponding relation for $j \neq 0$ is

$$f_{j,k} = - \frac{1}{2\pi i j} \int_0^1 e^{-2\pi i k \tau} \{f(1,\tau) - f(0,\tau)\}\, d\tau -$$

$$- \frac{1}{(2\pi i j)^2} \int_0^1 e^{-2\pi i k \tau} \{D_t f(1,\tau) - D_t f(0,\tau)\} +$$

$$+ \frac{1}{(2\pi i j)^2} \int_0^1 \int_0^1 e^{-2\pi i j t - 2\pi i k \tau} D_t^2 f(t,\tau)\, dt\, d\tau .$$

If both j and k are not zero one can write

$$f_{j,k} = -\frac{1}{2\pi ij} \int_0^1 e^{-2\pi ik\tau} \{f(1,\tau)-f(0,\tau)\}d\tau -$$

$$- \frac{1}{(2\pi ij)(2\pi ik)} \int_0^1 e^{-2\pi ijt} \{D_t f(t,1)-D_t f(t,0)\} +$$

$$+ \frac{1}{(2\pi ij)(2\pi ik)} \int_0^1\int_0^1 e^{-2\pi ijt-2\pi ik\tau} D_t D_\tau f(t,\tau)dtd\tau .$$

Of course, the corresponding results hold for g if $g \in C^2$.

Consider a periodic function f so that

$$(4) \qquad f(1,\tau) = f(0,\tau) ,$$

$$f(t,1) = f(t,0) .$$

The approximating smoothing spline g is not an unrestricted function minimizing (3). We assume that it also satisfies the corresponding boundary conditions

$$(5) \qquad g(1,\tau) = g(0,\tau)$$

$$g(t,1) = g(t,0)$$

and minimizes (3) among all such periodic functions. Let

$$\hat{x}_{j,k} = \frac{1}{n} \sum_{u,v=0}^{n-1} x_{u,v} \exp(-2\pi i(ju+kv)) ,$$

and

$$\tilde{g}_{j,k} = \sum_{u=v} g_{j+un,k+vn} \ .$$

Also, given the conditions (5), it follows that the Fourier coefficients

(6) $$(D_t g)_{j,k} = (2\pi i j) g_{jk}$$

$$(D_\tau g)_{jk} = (2\pi i k) g_{jk} \ .$$

The expression (3) can then be rewritten as

(7) $$\sum_{j,k=0}^{n-1} |\tilde{g}_{jk} - \frac{\hat{x}_{j,k}}{n}|^2 +$$

$$+ \lambda \sum_{j,k=0}^{n-1} \sum_{u,v=-\infty}^{\infty} \{ |j+un|^2 + |k+vn|^2 \} |g_{j+un,k+vn}|^2 \ .$$

The expression (7) can be minimized by separately minimizing the terms for each pair (j,k). A minimum is obtained for $(j,k) = (0,0)$ by setting

$$\tilde{g}_{00} = \frac{\hat{x}_{00}}{n} \ , \ g_{un,vn} = 0 \quad \text{if} \quad (u,v) \neq (0,0) \ .$$

This implies that

$$g_{0,0} = \frac{\hat{x}_{0,0}}{n} \ .$$

If $(j,k) \neq (0,0)$ we have

$$\left(\tilde{g}_{jk} - \frac{\hat{x}_{j,k}}{n}\right) + \lambda\{|j+un|^2 + |k+vn|^2\}g_{j+un,k+vn} = 0$$

and so

$$g_{j+un,k+vn} = -\frac{\left(\tilde{g}_{j,k} - \frac{\hat{x}_{j,k}}{n}\right)}{\lambda\{|j+un|^2 + |k+vn|^2\}} ,$$

$$\tilde{g}_{j,k} = -\left(\tilde{g}_{j,k} - \frac{\hat{x}_{jk}}{n}\right)\frac{1}{\lambda}r_{jk}$$

where

$$r_{jk} = \sum_{u,v}\frac{1}{\{|j+un|^2+|k+vn|^2\}} .$$

Consequently

$$g_{jk} = \frac{\hat{x}_{jk}}{n}\frac{r_{j,k}}{\lambda+r_{j,k}} , \quad j,k = 0,1,\ldots,n-1$$

and

$$g_{j+un,k+vn} = \frac{\hat{x}_{jk}}{n}\{|j+un|^2+|k+vn|^2\}^{-1}\frac{1}{\lambda+r_{j,k}} .$$

The expected integrated mean square error of $g(t,s;\lambda)$ as an estimate of f is

$$E\int_0^1\int_0^1 |g(t,s;\lambda) - f(t,s)|^2 dtds =$$

$$= E \sum_{j,k=-\infty}^{\infty} |g_{j,k} - f_{j,k}|^2$$

and

$$E|g_{j,k}-f_{j,k}|^2 = |Eg_{j,k}-f_{j,k}|^2 + \sigma^2(g_{j,k}) \ .$$

Now

$$\sigma^2(g_{0,0}) = \frac{\sigma^2}{n^2}$$

$$E\ g_{00} = \tilde{f}_{00} \ .$$

Since $g_{un,vn} = 0$ for $(u,v) \neq (0,0)$, $\sigma^2(g_{un,vn}) = 0$ for $(u,v) \neq (0,0)$. If $(j,k) \neq (0,0)$, $j,k = 0,1,\ldots,n-1$

$$E(\hat{x}_{j,k}/n) = \tilde{f}_{jk} \ .$$

For this range of (j,k) we have

$$E\ g_{j+un,k+vn} = \{|j+un|^2+|k+vn|^2\}^{-1}(\lambda+r_{jk})^{-1}\tilde{f}_{jk}$$

and

$$\sigma^2(g_{j+un,k+vn}) = \{|j+un|^2+|k+vn|^2\}^{-2}(\lambda+r_{jk})^{-2}\frac{\sigma^2}{n^2} \ .$$

THE RESULTS. The expected integrated mean square error is the sum of the integral of the variance of g , $\int \sigma^2[g(t,\tau)]dtd\tau$, and the integral of the bias of g

squared. Each of these terms will be estimated under assumptions which imply that they tend to zero as $n \to \infty$. The first result is concerned with the variance.

THEOREM 1. *Let* $f \in C$ *and satisfy the boundary conditions* (4). *If* g *minimizes* (3) *among all functions satisfying* (5), *then* $\int_0^1\int_0^1 \sigma^2[g(t,\tau)]\,dt\,d\tau \to 0$ *as* $n \to \infty$ *and* $\lambda(n) \to 0$ *if and only if* $\lambda(n)n^2 \to \infty$. *If this is so then*

$$\text{(8)}\quad \int_0^1\int_0^1 \sigma^2[g(t,\tau)]\,dt\,d\tau \cong \frac{\sigma^2}{n^2\lambda(n)} \int\int_{-\infty}^{\infty} \frac{dx\,dy}{(1+x^2+y^2)^2} + o(n^{-2}\lambda(n)^{-1}) \,.$$

The integral of $\sigma^2[g(t,\tau)]$ can be written as

$$\frac{\sigma^2}{n^2} + \frac{\sigma^2}{n^2} \sum_{j,k=0}^{n-1}{}' \sum_{u,v=-\infty}^{\infty} \{|j+un|^2+|k+vn|^2\}^{-2} (\lambda+r_{jk})^{-2}$$

where $\sum'$ denotes the sum deleting $(j,k)=(0,0)$. This can in turn be shown to be equal to

$$\frac{\sigma^2}{n^2} + \frac{\sigma^2}{n^2} \sum_{|j|,|k|\le\frac{n}{2}}{}' (\lambda+r_{jk})^{-2} \sum_{u,v=-\infty}^{\infty} \{|j+un|^2+|k+vn|^2\}^{-2} +$$

$$+\ O(\lambda^{-2}n^{-6}) \,.$$

The sum can be written as

$$\frac{\sigma^2}{n^2} + \frac{\sigma^2}{n^2} \sum_{|j|,|k|\le\frac{n}{2}}{}' (\lambda+r_{jk})^{-2} \left(\frac{1}{(j^2+k^2)^2} + e_{jk}\right) =$$

$$= \frac{\sigma^2}{n^2} \sum_{|j|,|k|\le\frac{n}{2}}' (\lambda+r_{jk})^{-2} \frac{1}{(j^2+k^2)^2} + R$$

with the term $e_{jk} = O(n^{-4})$ uniformly in j,k and so

$$R = O\left\{ n^{-6} \sum_{|j|,|k|\le\frac{n}{2}} \frac{1}{(\lambda+r_{jk})^2} \right\} = O(n^{-4}\lambda^{-2}) .$$

Also

$$\frac{1}{(j^2+k^2)^2} \frac{1}{(\lambda+r_{jk})^2} = \frac{1}{(1+\lambda(j^2+k^2))^2} + d_{jk}$$

with

$$|d_{jk}| \le \frac{K}{(1+\lambda(j^2+k^2))} (j^2+k^2)\left[\{(j+n)^2+k^2\}^{-1} + \{j^2+(k+n)^2\}\right]^{-1}$$

and K a constant. Now

$$\frac{\sigma^2}{n^2} \sum_{|j|,|k|\le\frac{n}{2}}' |d_{jk}| \le$$

$$\le \frac{\sigma^2}{n^4} \sum_{|j|,|k|\le\frac{n}{2}}' \frac{(j^2+k^2)}{(1+\lambda(j^2+k^2))^3} =$$

$$= O(n^{-4}\lambda^{-1}) .$$

Since

$$\frac{\sigma^2}{n^2}\sum_{|j|,|k|\le\frac{n}{2}}\frac{1}{(1+\lambda(j^2+k^2))}\cong$$

$$\cong\frac{\sigma^2}{n^2\lambda}\int_{-\infty}^{\infty}\int\frac{dxdy}{(1+x^2+y^2)^2}$$

the theorem follows.

Let us note that if $f\in C^3$ and satisfies the boundary conditions (4), the following asymptotic estimates hold for the Fourier coefficients f_{jk} :

(9') $$f_{jk}=-\frac{1}{(2\pi ij)^2}a_k+o\left(\frac{1}{j^2}\right)$$

as $|j|\to\infty$ with

$$a_k=\int_0^1 e^{-2\pi ik\tau}\{D_tf(1,\tau)-D_tf(0,\tau)\}d\tau\ ,$$

(9") $$f_{jk}=-\frac{1}{(2\pi ik)^2}b_j+o\left(\frac{1}{k^2}\right)$$

as $|k|\to\infty$ with

$$b_j=\int_0^1 e^{-2\pi ijt}\{D_\tau f(t,1)-D_\tau f(t,0)\}dt\ ,$$

(9"') $$f_{jk}=\frac{1}{(2\pi ij)^2}\frac{1}{(2\pi ik)^2}\left[(D_tD_\tau f(1,\tau)-D_tD_\tau f(0,\tau))\Big|_0^1-\right.$$

$$\left.-(D_t^2D_\tau f(t,1)-D_t^2D_\tau f(t,0))\Big|_0^1\right]+o\left(\frac{1}{j^2k^2}\right)$$

as $|j|,|k| \to \infty$. This suggests considering the following more general set of conditions:

(10') $$|f_{jk}|^2 = |j|^{-2\eta}|a_k|^2 + o(|j|^{-2\eta})$$

as $|j| \to \infty$,

(10") $$|f_{jk}|^2 = |k|^{-2\eta}|b_j|^2 + o(|k|^{-2\eta})$$

as $|k| \to \infty$,

(10"') $$|f_{jk}|^2 = \gamma|jk|^{-2\eta} + o(|jk|^{-2\eta})$$

as $|j|,|k| \to \infty$, all with $\frac{5}{2} > \eta > \frac{1}{2}$.

THEOREM 2. *If* $\lambda \to 0$ *and* $n^2\lambda \to \infty$ *as* $n \to \infty$ *, then under the assumption that*

(11)
$$f_{jk} = O(j^{-1-\varepsilon}) \quad \text{as} \quad |j| \to \infty$$
$$f_{jk} = O(k^{-1-\varepsilon}) \quad \text{as} \quad |k| \to \infty$$
$$f_{jk} = O((jk)^{-1-\varepsilon}) \quad \text{as} \quad |j|,|k| \to \infty$$

for some $\varepsilon > 0$ *, we have the integrated squared bias*

(12) $$\int_0^1 \int_0^1 |Eg(t,\tau) - f(t,\tau)|^2 dt d\tau =$$

$$= \sum_{|j|,|k| \le \frac{n}{2}} |f_{jk}|^2 \frac{\lambda^2 (j^2+k^2)^2}{(1+\lambda(j^2+k^2))^2} +$$

$$+ O(n^{-4}\lambda^{-2\epsilon} + n^{-2-2\epsilon}\lambda^{-1} + n^{-1}) \ .$$

Under the condition (10) *the integrated squared bias is*

$$(13) \qquad \cong \lambda^{\eta-\frac{1}{2}} \left\{ \sum |a_k|^2 + \sum |b_k|^2 \right\}$$

$$\int \frac{x^{4-2\eta}}{(1+x^2)^2}\, dx$$

as $n \to \infty$. *In the special case of condition* (9) *we have*

$$(14) \qquad \sum |a_k|^2 = \int_0^1 |D_t f(1,\tau) - D_t f(0,\tau)|^2 \, dt$$

and

$$(14') \qquad \sum |b_k|^2 = \int_0^1 |D_\tau f(t,1) - D_\tau f(t,0)|^2 \, dt \ .$$

First notice that the integrated squared bias can be written as

$$|f_{00} - \tilde{f}_{00}|^2 + \sum_{j,k=0}^{n-1}{}' \sum_{u,v} \left| \frac{\tilde{f}_{jk}}{\{(j+un)^2 + (k+vn)^2\}(\lambda + r_{jk})} - f_{jk} \right|^2 \ .$$

Our object is to approximate this expression by

$$(15) \qquad \sum_{|j|,|k| \le \frac{n}{2}} \left| \frac{f_{jk}}{(j^2+k^2)(\lambda + r_{jk})} - f_{jk} \right|^2 \ .$$

Using

$$\tilde{f}_{jk} = f_{jk} + (\tilde{f}_{jk} - f_{jk})$$

the error in the approximation can be seen to be of the order of

$$(16) \quad |f_{00} - \tilde{f}_{00}|^2 + \sum_{j,k=0}^{n-1}{}' \sum_{\substack{|j+un|>\frac{n}{2} \\ \text{or} \\ |k-un|>\frac{n}{2}}} \frac{|\tilde{f}_{jk}|^2}{\{(j+un)^2+(k+vn)^2\}^2 (\lambda+r_{jk})^2} +$$

$$+ \sum_{\substack{|j|>\frac{n}{2} \\ \text{or} \\ |k|>\frac{n}{2}}} |f_{jk}|^2 + \sum_{j,k=0}^{n-1} \sum_{\substack{|j+un|\le\frac{n}{2} \\ \text{or} \\ |k+vn|\le\frac{n}{2}}} \frac{|\tilde{f}_{jk} - f_{jk}|^2}{\{(j+un)^2+(k+vn)^2\}(\lambda+r_{jk})} .$$

The first term of (16) is $O(n^{-4})$. The third term of (16) can be shown to be $O(n^{-1-2\epsilon})$. The second term of (16) is

$$O\left(n^{-4} \sum_{j,k=0}^{n-1} \frac{|\tilde{f}_{jk}|^2}{(\lambda+r_{jk})^2} \right) .$$

Under the assumption (11) this can be seen to be $O(n^{-4}\lambda^{-2+\epsilon})$. The last term of (14) can be estimated by

$$O(n^{-2-2\epsilon}\lambda^{-1}) .$$

It is useful in estimating (15) to remark that

$$\frac{1}{(j^2+k^2)(\lambda+r_{jk})} = \frac{1}{1+\lambda(j^2+k^2)} \left\{1 + O\left[\frac{j^2+k^2}{(j+n)^2+k^2} + \frac{j^2+k^2}{j^2+(k+n)^2}\right]\right\} .$$

This implies that (15) equals

$$(17) \qquad \sum_{|j|,|k|\le\frac{n}{2}}' |f_{jk}|^2 \frac{\lambda^2 (j^2+k^2)}{(1+\lambda(j^2+k^2))^2} +$$

$$+ C \left\{ \sum_{|j|,|k|\le\frac{n}{2}} |f_{jk}|^2 \left[\frac{(\frac{j}{n})^2+(\frac{k}{n})^2}{(\frac{j}{n}+1)^2+(\frac{k}{n})^2} + \frac{(\frac{j}{n})^2+(\frac{k}{n})^2}{(\frac{j}{n})^2+(\frac{k}{n}+1)^2}\right]\right\} .$$

The second term of (17) is clearly $O(n^{-1-2\epsilon})$. This gives us the estimate (12). If the asymptotic behavior of the Fourier coefficients f_{jk} is prescribed by conditions (10),

$$\sum_{|j|\le\frac{n}{2}} |f_{jk}|^2 \frac{\lambda^2(j^2+k^2)^2}{1+\lambda(j^2+k^2))^2}$$

for fixed k is asymptotically the same as

$$\lambda^2 |a_k|^2 \sum_{|j|\le\frac{n}{2}} \frac{|j|^{4-2n}}{(1+\lambda j^2)^2} \cong \lambda^{n-\frac{1}{2}} \int \frac{x^{4-2n}}{(1+x^2)^2} dx |a_k|^2 .$$

This and the corresponding result for $\sum_{|k|\le\frac{n}{2}} |f_{jk}|^2$

with j fixed lead to (13). When $n=1$ (14) and (14') are obtained.

COROLLARY 1. *If*

$$\sum_{j,k} |f_{jk}|^2 (j^2+k^2)^2 < \infty \tag{18}$$

the integrated squared bias is asymptotically to the first order

$$\lambda^2 \sum_{j,k} |f_{jk}|^2 (j^2+k^2)^2 .$$

This remark follows immediatley from Theorem 2. Notice that for a function $f \in C^3$, the condition (18) will be satisfied only if the boundary conditions

$$D_t f(1,\tau) = D_t f(0,\tau) , \tag{19}$$

$$D_\tau f(t,1) = D_\tau f(t,0)$$

are satisfied in addition to (4).

If (18) is satisfied, the optimal rate of decay to zero for the integrated mean square error is $n^{-4/3}$ and this occurs when $\lambda(n) \sim n^{-2/3}$. If the conditions (9) are satisfied the optimal rate is $n^{-6/5}$ and this is obtained when $\lambda(n) \sim n^{-4/5}$. Notice that this slower rate is due to a boundary effect just as in the one dimensional

case, the fact that the boundary conditions (19) are not satisfied.

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Murray Rosenblatt
University of California, San Diego
La Jolla, California 92093
U.S.A.

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Two-dimensional, smoothing spline, regression, boundary effects.

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A two-dimensional analogue of a smoothing spline problem is considered. It is shown how boundary effects can arise here even in the case of periodicity. Additional keywords: naval research, Fourier analysis, coefficients, approximation (mathematics).

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